Uncertainty Quantification Tools for Multiphase Flow Simulations using MFIX

Formulation of an Uncertainty Quantification Approach Based on Direct Quadrature Sampling of the Parameter Space

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University Coal Research and Historically Black Colleges and Universities and Other Minority Institutions Contractors Review Conference

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Outline

Outline

Background and motivations

Eulerian multiphase models for gas-particle flows

- Widely used in both academia and industry
- Computationally efficient
- Applicable to real-world cases (gasifiers, combustors, ...)
- Directly provide averaged quantities of interest in design and optimization studies

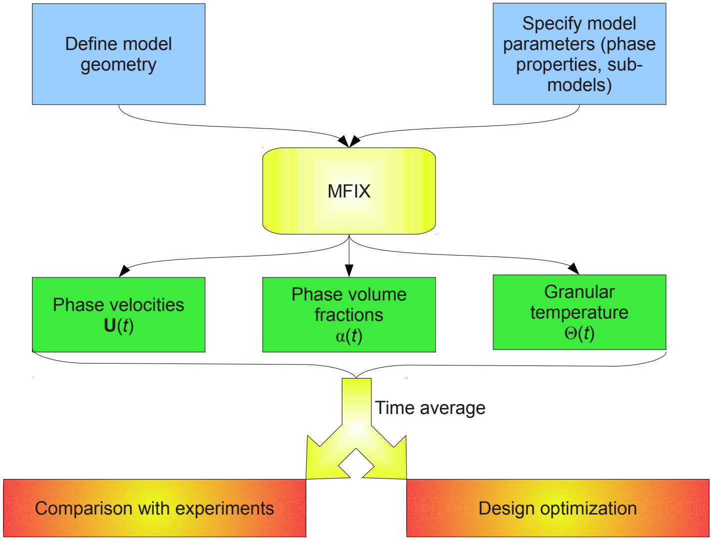
Need of uncertainty quantification

- Study how the models propagate uncertainty from inputs to outputs

Main objectives

- Develop an efficient quadrature-based uncertainty quantification procedure
- Apply such a procedure to multiphase gas-particle flow simulations considering parameters of interest in applications

Typical steps in a simulation project with MFIX



Models and uncertainty

- Models present a strongly non-linear relation between inputs and outputs
- Input parameters are affected by uncertainty
    - Experimental inputs
        - Experimental errors
        - Difficult measurements
    - Theoretical assumptions
        - Model assumptions might introduce uncertainty
- Need to quantify the effect of uncertainty on the simulation results
    - Uncertainty propagation from inputs to outputs of the model
    - Multiphase models are complex: non-intrusive approach
        - Generate a set of samples of the results of the original models
        - Use the information collected from samples to calculate statistics of the system response
        - Key element is the sampling procedure: efficiency

Outline

Project tasks

Uncertainty quantification tools for multiphase gas-solid flow simulations using MFIX

- **Task 1.0 Project management plan**
- **Task 2.0 Formulation of robust non-intrusive quadrature-based UQ approach**
  - ***Task 2.1 Formulation of the quadrature-based UQ procedure***
  - ***Task 2.2 Validation on a set of simplified test cases***
- **Task 3.0 Implementation of the quadrature-based procedure into MFIX**
  - ***Task 3.1 Implementation of the quadrature-based UQ algorithm***
  - ***Task 3.2 Development of tools for automated sample processing and data post-processing***
- **Task 4.0 Application to gas-particle flow test cases**
  - ***Task 4.1 Development of a validation criterion for MFIX simulations***
  - ***Task 4.2 UQ on bubbling fluidized bed simulations***
  - ***Task 4.3 UQ on r iser flow simulations***

Project milestones and current status

Milestone n.	Description	Due on	Status
1	Submission of project management plan	Dec. 30, 2011	Completed
2	Formulation of the quadrature-based UQ procedure	Jul. 1, 2012	On time
3	Validation of the quadrature-based UQ procedure on simplified test-cases	Oct. 1, 2012	Starts on Jul. 2, 2012
4	Implementation of the quadrature-based UQ algorithm into MFIX	May 31, 2013	Starts on Oct. 2, 2012
5	Development of automated tools for processing input/output data	Oct. 1, 2013	Starts on May 3, 2013
6	Development of a Validation Criterion for MFIX Simulations	Jan. 3, 2014	Starts on Oct. 10, 2013
7	UQ on bubbling fluidized bed simulations	Mar. 31, 2014	Starts on Oct. 10, 2013
8	UQ on riser flow simulations	Sept. 1, 2014	Starts on Apr. 1, 2014
9	Preparation of final report	Sept 31, 2014	Starts on Sept. 1, 2014

Outline

Basic concepts

- We study propagation of uncertainty from inputs to outputs
- The distribution of the values (PDF) of the uncertain parameters is assumed to be known
  - Uniform
  - Gaussian
  - ...
- The moments (statistics) of the model results are the quantity of interest
  - Low-order statistics for practical purposes (mean, variance, ...)
  - PDF of the response

Quadrature-based uncertainty quantification - 1D case

- We start considering a simplified case
  - Probability space $\mathcal{P}(\Omega, \mathcal{F}, P)$, with Ω a sample space, $\mathcal{F}$ a σ-algebra and P a probability measure.
  - One random variable (uncertain parameter) ξ
  - A random process $u(\xi, x)$ (our model)
- The objective is to compute the moments of the random process:

$$m_n = \int_{\Omega} u(\xi, x)^n p(\xi) \mathrm{d}\xi$$

Direct quadrature approach

- Sample Ω using Gaussian quadrature formulae
- Evaluate the model in correspondence of each quadrature node (find abscissas)
- Approximate moments directly in terms of the quadrature weights and abscissas

Quadrature-based uncertainty quantification - 1D case

- If $p(\xi)$ is considered as the weight function of a Gaussian quadrature formula, the moments about the origin of the response can be approximated as

$$m_n = \int_\Omega u(\xi, x)^n p(\xi) \mathrm{d}\xi = \sum_{i=1}^{\mathrm{M}} w_i(x) \left[u(\xi_i, x)\right]^n$$

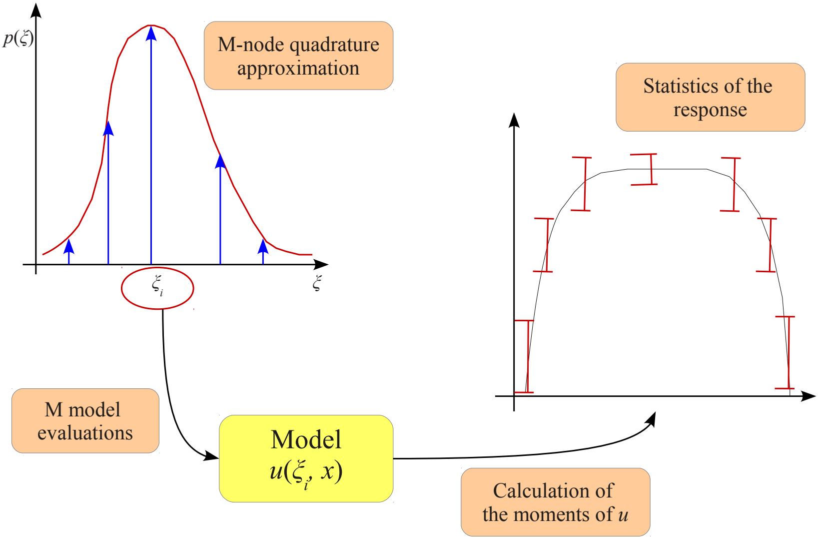
being

- M the number of nodes
- $w_i(x)$ the quadrature weights
- ξ_i the quadrature nodes

Weight functions

The form of $p(\xi)$ depends on the assumed probability distribution function of the uncertain parameter (uniform, Gaussian, ...)

Summary of the 1D procedure



Quadrature-based UQ - Multivariate case

- We consider now a multi-variate case:
  - N uncertain parameters $\boldsymbol{\xi} = \{\xi_1, \xi_2, \ldots, \xi_\mathrm{N}\}$
  - Joint PDF $p(\xi_1, \xi_2, \ldots, \xi_\mathrm{N})$
- The moments of the response u are then

$$\langle u^n(\boldsymbol{\xi})\rangle = \int_{\mathbb{R}^\mathrm{N}} [u(\boldsymbol{\xi})]^n p(\boldsymbol{\xi}) \mathrm{d}\boldsymbol{\xi}$$

Conditional probability

- The joint PDF can be re-written in terms of conditional PDF's as

$$p(\xi_1, \ldots, \xi_\mathrm{N}) = p(\xi_\mathrm{N}|\xi_1, \ldots, \xi_\mathrm{N\text{-}1}) p(\xi_\mathrm{N\text{-}1}|\xi_1, \ldots, \xi_\mathrm{N\text{-}2}) \cdot \ldots \cdot p(\xi_2|\xi_1) p(\xi_1)$$

- It degenerates in the product of the marginal PDF's in the case of independent variables.

Quadrature-based UQ - Multivariate case

- We consider a case with three $(N = 3)$ random variables $\boldsymbol{\xi} = \xi_1, \xi_2, \xi_3$.
- The joint PDF is

$$p(\xi_1, \xi_2, \xi_3) = p(\xi_3|\xi_1, \xi_2)p(\xi_2|\xi_1)p(\xi_1)$$

Conditional moments

$$\langle \xi_3^k \rangle(\xi_1, \xi_2) = \int_{\mathbb{R}} \xi_3^k p(\xi_3|\xi_1, \xi_2)\mathrm{d}\xi_3 \quad \langle \xi_2^j \rangle(\xi_1) = \int_{\mathbb{R}} \xi_2^j p(\xi_2|\xi_1)\mathrm{d}\xi_2$$

Pure moments

$$m_{i,j,0} = \int_{\mathbb{R}^2} \xi_1^i \xi_2^j p(\xi_1, \xi_2)\mathrm{d}\xi_1\mathrm{d}\xi_2 = \int_{\mathbb{R}} \xi_1^i \langle \xi_2^j \rangle(\xi_1) p(\xi_1)\mathrm{d}\xi_1\xi_3$$

$$m_{i,j,k} = \int_{\mathbb{R}^3} \xi_1^i \xi_2^j \xi_3^k p(\xi_1, \xi_2, \xi_3)\mathrm{d}\xi_1\mathrm{d}\xi_2\mathrm{d}\xi_3 = \int_{\mathbb{R}^2} \xi_1^i \xi_2^j \langle \xi_3^k \rangle(\xi_1, \xi_2) p(\xi_1, \xi_2)\mathrm{d}\xi_1\mathrm{d}\xi_2$$

Conditional quadrature approximation

1. Use M_1-point 1-D quadrature to sample ξ_1:

$$p(\xi_1) = \sum_{l_1=1}^{M_1} n_{l_1} \delta(\xi_1 - \xi_{1,l_1})$$

   - Weights n_{l_1} and nodes ξ_{1,l_1}
2. Find the conditional moments

$$\langle \xi_2^j \rangle_{l_1}, j = 1, \ \ldots, 2M_2 - 1, \ \forall l_1$$

   - Use M_2-point 1-D quadrature to find weights n_{l_1,l_2} and nodes ξ_{2,l_1,l_2}
3. Find the conditional moments

$$\langle \xi_3^k \rangle_{l_1,l_2}, \ k = 1, \ldots, 2M_3 - 1 \ \forall l_1, l_2$$

   - Use M_3-point 1-D quadrature to find weights n_{l_1,l_2,l_3} and nodes ξ_{3,l_1,l_2,l_3}

Conditional quadrature approximation

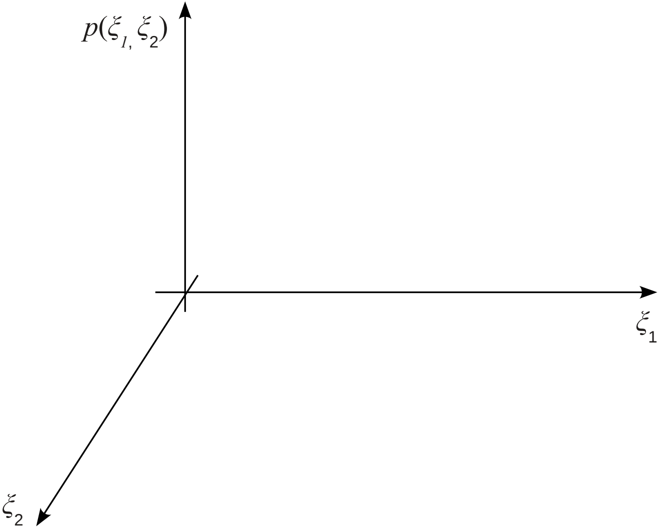
- The joint PDF is then approximated as:

$$p(\boldsymbol{\xi}) = \sum_{l_1=1}^{M_1} \sum_{l_2=1}^{M_2} \sum_{l_3=1}^{M_3} n_{l_1} n_{l_1,l_2} n_{l_1,l_2,l_3} \delta(\xi_1 - \xi_{1,l_1}) \delta(\xi_2 - \xi_{2,l_1,l_2}) \delta(\xi_3 - \xi_{3,l_1,l_2,l_3})$$

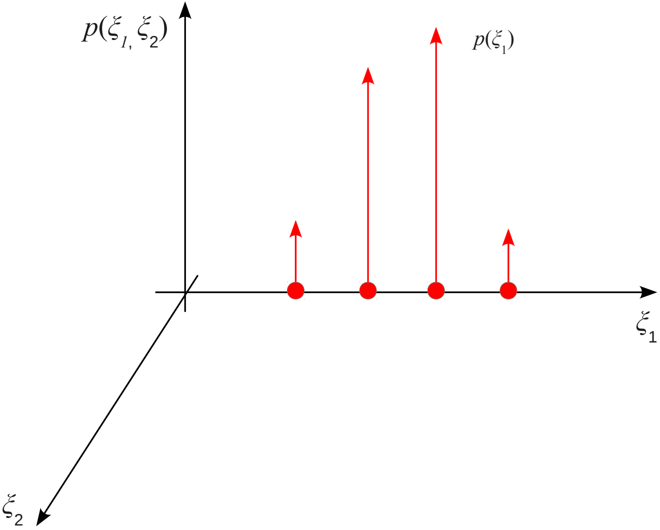
- The moments of the system response are computed as:

$$\begin{aligned} \langle u^n(\boldsymbol{\xi}) \rangle &= \int_{\mathbb{R}^3} [u(\boldsymbol{\xi})]^n p(\boldsymbol{\xi}) \mathrm{d}\boldsymbol{\xi} \\ &= \sum_{l_1=1}^{M_1} \sum_{l_2=1}^{M_2} \sum_{l_3=1}^{M_3} n_{l_1} n_{l_1,l_2} n_{l_1,l_2,l_3} \left[u(\xi_{1,l_1}, \xi_{2,l1,l2}, \xi_{3,l1,l2,l3}) \right]^n \end{aligned}$$

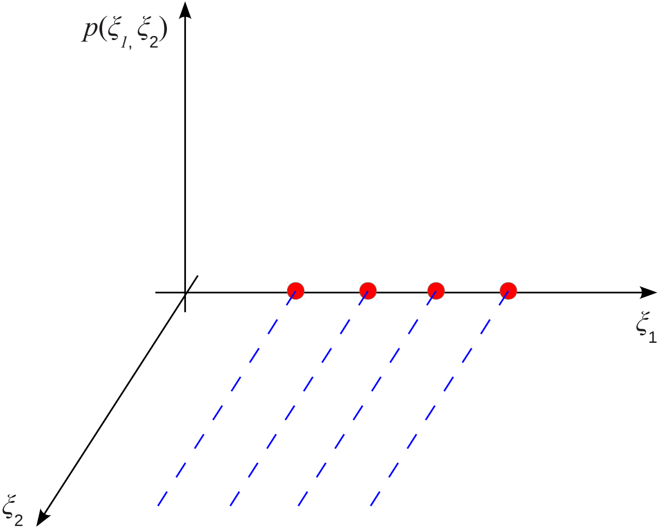
Quadrature-based UQ - Visualization of a bivariate case



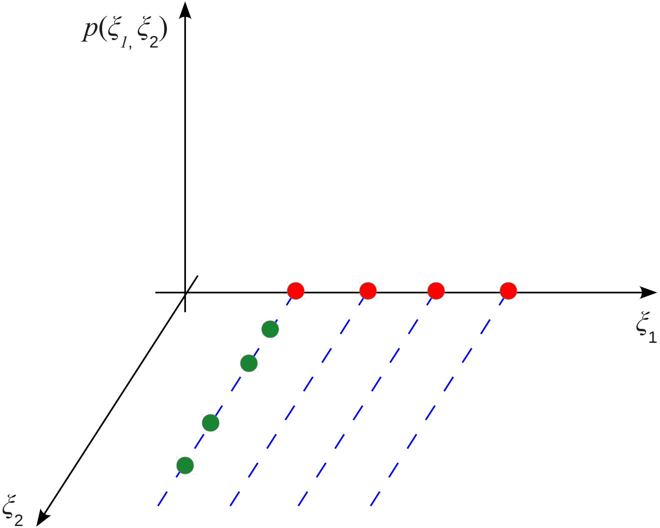
Quadrature-based UQ - Visualization of a bivariate case



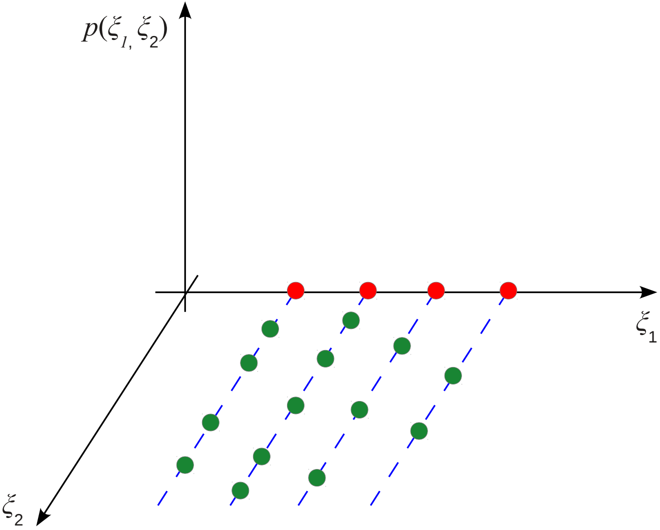
Quadrature-based UQ - Visualization of a bivariate case



Quadrature-based UQ - Visualization of a bivariate case



Quadrature-based UQ - Visualization of a bivariate case



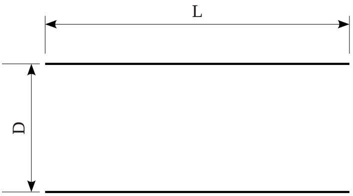
Summary: Quadrature-based uncertainty quantification

- Multivariate sampling method for the joint-PDF of the input parameters
  - Degenerates in 1D quadrature if only one uncertain parameter is considered
  - Falls back to a traditional tensor product if the uncertain parameters are independent
- Equivalent to stochastic collocation (Yoon at al., 2010, AIAA 2010-8171)
- High-order convergence of the moments of the response

Example applications

- Objectives
  - Validate the UQ procedure with simple test cases
  - Study the convergence of the moments of the response in cases of interest
- Test cases
  - Developing channel flow
    - Simple test case from the literature
    - Reference results
    - Low computational cost: convergence study
  - Oblique shock problem
    - Discontinuous solution (typical in multiphase flows!)
    - Performance of the procedure in presence of discontinuities

Developing channel flow



Properties

- $L/D = 6$
- $\mathrm{Re} = DU/\nu_0 = 81.24$
- $\sigma(\nu) = 0.3\nu_0$
- Uniform inlet (Le Mâitre et. al., 2011)

- Mesh: 65 x 256 cells
- Steady state solution
- Convergence criterion: residuals below $1.0\text{x}10^{-12}$
- Incompressible solver: simpleFoam (OpenFOAM®)

Performed study

- Convergence of the moments:
  - Absolute error
  - Moments up to 9$^{\text{th}}$ order
- Statistics of the response

Convergence of the moments

- Absolute error $e_{\text{abs},n,i} = |m_{n,i} - m_{n,1000}|$, assuming the moments obtained with 1000 samples are exact.

Samples	$e_{\text{abs},0,i}$	$e_{\text{abs},1,i}$	$e_{\text{abs},2,i}$	$e_{\text{abs},3,i}$
3	4.440×10^{-16}	5.588×10^{-6}	8.646×10^{-5}	9.486×10^{-4}
5	7.771×10^{-16}	2.389×10^{-8}	2.184×10^{-7}	1.401×10^{-6}
10	5.551×10^{-16}	3.018×10^{-9}	3.064×10^{-8}	2.335×10^{-7}
20	4.440×10^{-16}	7.214×10^{-12}	2.036×10^{-11}	8.278×10^{-10}
40	8.881×10^{-16}	6.814×10^{-10}	6.813×10^{-9}	5.110×10^{-8}
60	9.992×10^{-16}	4.376×10^{-12}	7.179×10^{-11}	7.522×10^{-10}
80	8.881×10^{-16}	5.182×10^{-11}	5.152×10^{-10}	3.839×10^{-9}
100	7.771×10^{-16}	6.509×10^{-11}	6.531×10^{-10}	4.918×10^{-9}

Table: Absolute error of m_0, m_1, m_2 , m_3 as a function of the number of samples.

Convergence of the moments

Samples	$e_{\mathrm{abs},4,i}$	$e_{\mathrm{abs},5,i}$	$e_{\mathrm{abs},6,i}$
3	8.877×10^{-3}	7.542×10^{-2}	5.994×10^{-1}
5	6.990×10^{-6}	2.241×10^{-5}	4.571×10^{-5}
10	1.583×10^{-6}	1.007×10^{-5}	6.161×10^{-5}
20	9.895×10^{-9}	8.844×10^{-8}	6.855×10^{-7}
40	3.407×10^{-7}	2.130×10^{-6}	1.278×10^{-5}
60	6.465×10^{-9}	4.961×10^{-8}	3.539×10^{-7}
80	2.540×10^{-8}	1.574×10^{-7}	9.356×10^{-7}
100	3.295×10^{-8}	2.070×10^{-7}	1.250×10^{-6}

Table: Absolute error of m_4, m_5, m_6 as a function of the number of samples.

Convergence of the moments

Samples	$e_{\text{abs},7,i}$	$e_{\text{abs},8,i}$	$e_{\text{abs},9,i}$
3	4.534×10^{0}	3.300×10^{1}	2.328×10^{2}
5	1.718×10^{-3}	2.107×10^{-2}	2.029×10^{-1}
10	3.667×10^{-4}	2.139×10^{-3}	1.230×10^{-2}
20	4.876×10^{-6}	3.271×10^{-5}	2.104×10^{-4}
40	7.463×10^{-5}	4.268×10^{-4}	2.402×10^{-3}
60	2.398×10^{-6}	1.565×10^{-5}	9.920×10^{-5}
80	5.399×10^{-6}	3.049×10^{-5}	1.692×10^{-4}
100	7.341×10^{-6}	4.226×10^{-5}	2.397×10^{-4}

Table: Absolute error of m_7, m_8, m_9 as a function of the number of samples.

Conclusions

- Mean and variance rapidly converge (less than 10 samples).
- Twenty samples provide the best trade-off in terms of moments convergence and efficiency for this case

Low-order statistics

- Variance (Distance from the mean)

$$\sigma^2 = \frac{m_2}{m_0} - \mu^2,$$

- Skewness (Symmetry of the distribution)

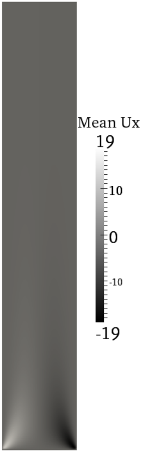
$$\gamma_1 = \frac{\mu_3}{\sigma^3} = \frac{m_3/m_0 - 3\mu m_2/m_0 + 2\mu^3}{\sigma^3},$$

- Kurtosis (Importance of tails)

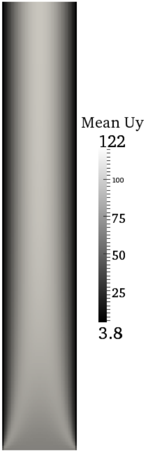
$$\gamma_2 = \frac{\mu_4}{\sigma^4} = \frac{m_4/m_0 - 4\mu m_3/m_0 + 6\mu^2 m_2/m_0 - 3\mu^4}{\sigma^4}.$$

- μ_i: central moments
- m_i: moments about the origin

Velocity mean

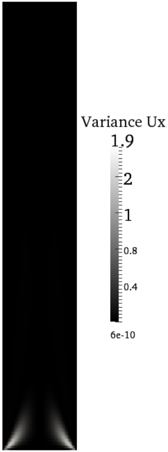


$\mu(U_x)$

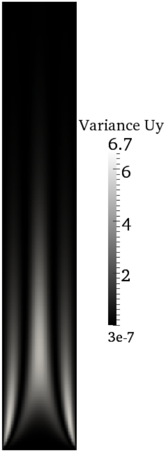


$\mu(U_y)$

Velocity variance

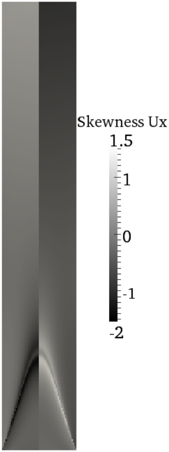


$\sigma^2(U_x)$

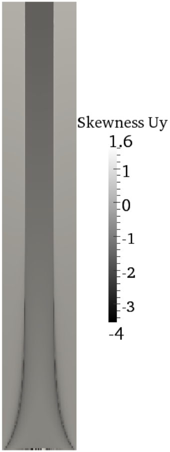


$\sigma^2(U_y)$

Velocity skewness

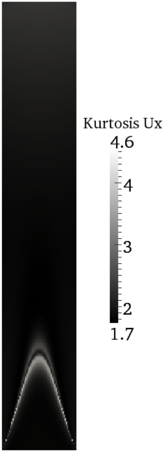


$\gamma_1(U_x)$

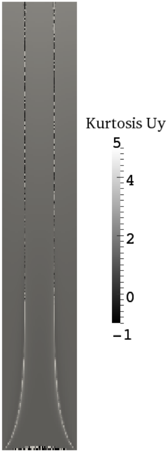


$\gamma_1(U_y)$

Velocity kurtosis

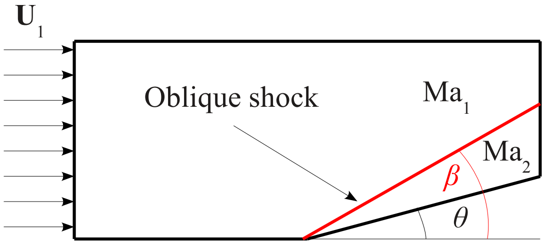


$\gamma_2(U_x)$



$\gamma_2(U_y)$

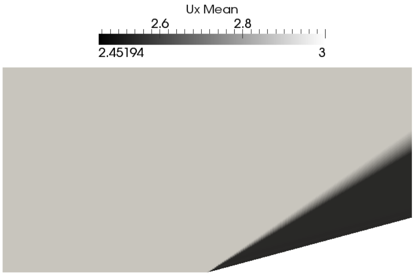
The oblique shock problem



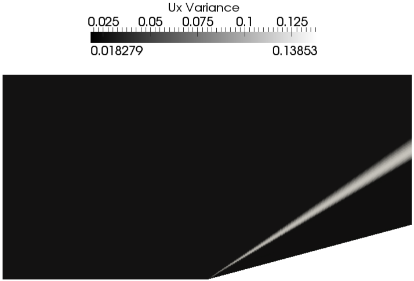
- $\mathrm{Ma} = |\mathbf{U}|/a = 3$
- $\mathrm{Ma} \in [2.7, 3.3]$
- $\tan\theta = 2\cot\beta \frac{\mathrm{Ma}_1^2 \sin^2\beta - 1}{\mathrm{Ma}_1^2(\gamma + \cos(2\beta) + 2}$

- Mesh: 640 x 320 cells
- Unsteady simulation (max CFL = 0.2)
- Compressible solver: rhoCentralFoam (OpenFOAM®)

Low-order statistics



$\mu(U_x)$

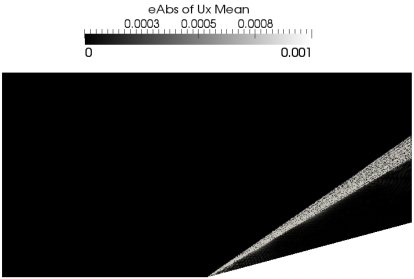


$\sigma^2(U_x)$

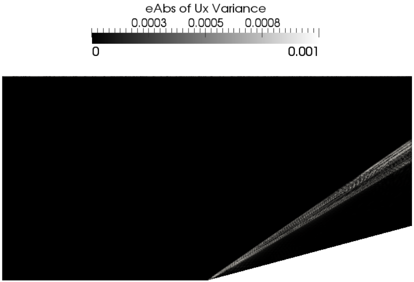
Ma_1	$\beta_{Analytical}$	β_{UQ}
2.7	34.78	34.32
3.3	30.27	30.50

Table: Analytical and UQ prediction of the shock angle - 20 samples

Absolute error of the statistics - 20 samples



$$|\mu(U_x)_{20} - \mu(U_x)_{100}|$$



$$|\sigma^2(U_x)_{20} - \sigma^2(U_x)_{100}|$$

Outline

Future work

- Reconstruction of the PDF of the system response (in progress)
- Validation of the quadrature-based UQ procedure on a set of simplified test-cases (in progress)
- Implementation of the procedure in suitable form to be used with MFIX
- Development of automation tools
- Applications to gas-particle flow in fluidized beds and risers

Personnel and publications

Personnel

- 1 Post-doc (Alberto Passalacqua) from October 2011
- 1 Ph.D. student (Xiaofei Hu) from June 2012

Publications

- A. Passalacqua, P. Vedula, R.O. Fox, A quadrature-based uncertainty quantification procedure with applications to computational fluid dynamics, In preparation.

Thanks for your attention!

Questions?